Supplementary Material (ESI) for Chemical Communications

A Highly Conformationally Specific α- and β-Ala$^+$ Decarboxylation Pathway

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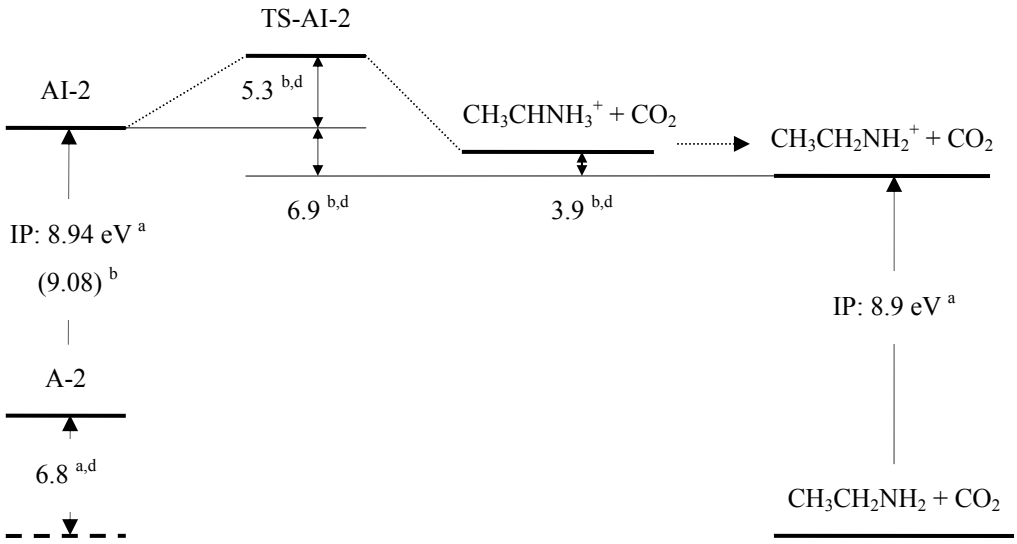
The energetic diagram of the decarboxylation of cationic Ala (Fig.1)



a: experimental value, b: calculated value,

c: Thermochemical data at 298 K (ref.14), d: kcal mol^{-1}

Geometry (Cartesian Coordinate, Unit: Angstrom)

AI-2 (Fig.1)

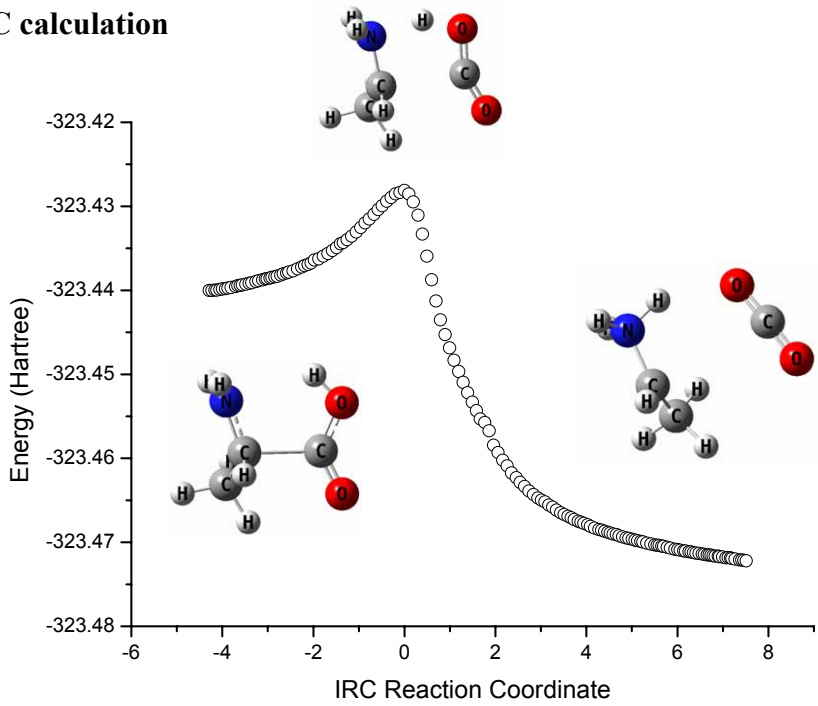
N	-1.252849	1.229016	0.148119
C	-0.780761	-0.038986	0.412712
H	-1.330075	1.928110	0.881527
H	-1.750469	1.425535	-0.716835
C	0.952279	-0.099441	0.058255
H	-0.712905	-0.225763	1.488959
O	1.502621	0.997438	-0.376238
O	1.465352	-1.152250	0.262565
H	0.855934	1.722147	-0.470652
C	-1.397951	-1.170877	-0.396039

H	-1.345429	-0.986637	-1.474189
H	-0.882520	-2.107649	-0.178149
H	-2.449773	-1.264537	-0.107682

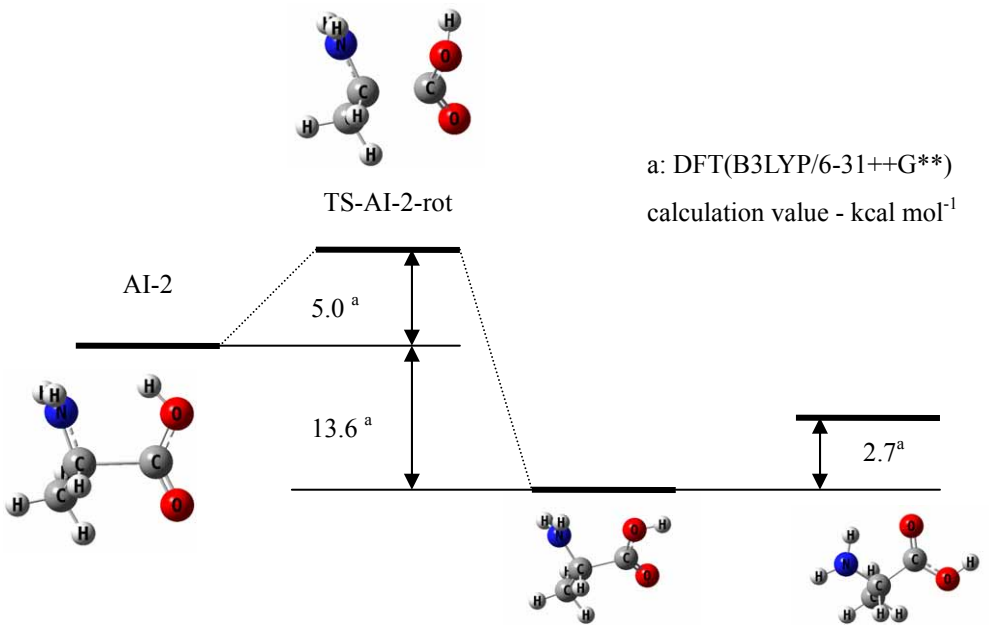
TS-AI-2(Fig.1)

N	-1.184954	1.203460	0.124147
C	-0.979718	-0.140646	0.485152
H	-1.416949	1.835908	0.891528
H	-1.807030	1.352646	-0.671976
C	1.258530	-0.056302	0.002028
H	-0.804382	-0.310848	1.545462
O	1.244846	1.126100	-0.380239
O	1.795394	-1.068393	0.216812
H	0.193484	1.468440	-0.269666
C	-1.488368	-1.241279	-0.372915
H	-0.953577	-2.173174	-0.175593
H	-2.548188	-1.420582	-0.125304
H	-1.433260	-1.008907	-1.441653

IRC calculation



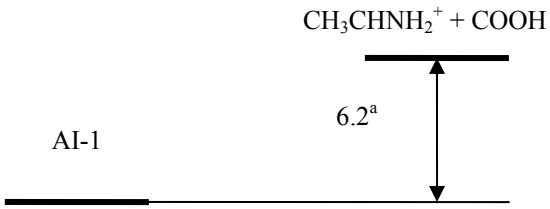
- Interconversion between two major conformers in cationic alanine

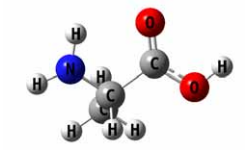


Geometry of TS-AI-2-rot (Cartesian Coordinate, Unit: Angstrom)

N	0	-1.034192	1.405926	-0.140786
C	0	-0.736959	0.157191	0.367607
H	0	-0.712889	2.259704	0.307236
H	0	-1.601823	1.508308	-0.978542
C	0	0.900836	-0.250805	-0.005197
H	0	-0.573144	0.214952	1.455272
O	0	1.741016	0.774513	0.074226
O	0	1.130832	-1.407184	-0.110514
H	0	1.820065	1.307330	-0.736582
C	0	-1.661379	-0.963021	-0.071117
H	0	-1.719329	-1.038773	-1.161502
H	0	-1.300426	-1.916748	0.316127
H	0	-2.662896	-0.775073	0.326044

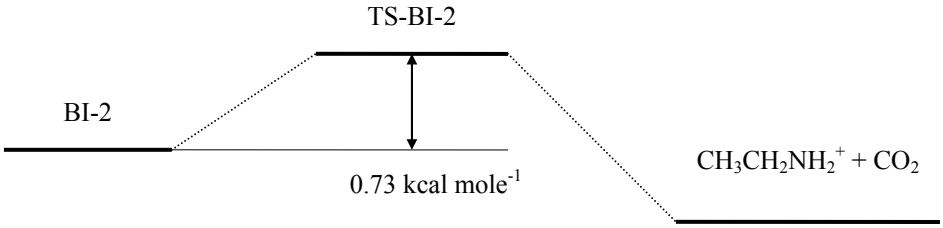
- COOH dissociation from AI-1





a: DFT(B3LYP/6-31++G**)
calculation value - kcal mol^{-1}

-Reaction Coordinate of β-Ala



Geometry (Cartesian Coordinate, Unit: Angstrom)

BI-2 (Fig. 2)

C	0.037037	1.047854	0.229911
H	0.412303	1.968190	-0.230140
H	-0.020757	1.242956	1.308978
C	-1.336702	0.722116	-0.367885
H	-1.275024	0.581511	-1.448930
H	-2.057864	1.512255	-0.153577
N	-1.882457	-0.581127	0.194052
H	-2.117694	-0.508186	1.189403
H	-2.723947	-0.887034	-0.304720
C	1.017059	-0.092610	0.011150
O	2.282193	0.198829	-0.003545
O	0.690705	-1.275354	-0.127131

H	-1.127360	-1.293763	0.086969

TS-BI-2 (Fig. 2)

C	-0.003378	1.073501	0.312179
H	0.458834	1.977799	-0.076891
H	-0.006445	1.052250	1.404437
C	-1.308686	0.751639	-0.373677
H	-1.184495	0.634720	-1.452822
H	-2.023689	1.564002	-0.197751
N	-1.916401	-0.535237	0.140612
H	-2.245467	-0.453427	1.108212
H	-2.706586	-0.842007	-0.435357
C	1.199675	-0.269547	-0.011043
O	2.259043	0.303387	-0.075139
O	0.609930	-1.337089	-0.050614
H	-1.154796	-1.250622	0.107151

IRC calculation